

- 1. A crystal of IMPDH (ionisine monophosphate dehydrogenase) isolated from a bacterial preparation.
- 2. The crystal of claim 1 further characterized by ability to provide x-ray diffraction patterns useful to define molecular structures for bacterial IMPDH enzymes.
- 3. A crystal of IMPDH (ionisine monophosphate dehydrogenase) isolated from a bacterial preparation wherein the bacterial preparation is a pure culture of *Streptococcus* pyogenes.
- 4. A method for designing inhibitors of bacterial IMPDH (inosine monophosphate dehydrogenase), said method comprising:
  - a. obtaining a crystal of bacterial IMPDH;
  - b. recording x-ray diffraction data from said crystal;
  - c. using said diffraction data to generate an electron density map consistent with a model for the molecular structure of a binding pocket of IMPDH; and
  - d. designing inhibitors of bacterial IMPDH based on the map of three dimensional structural information of the molecular structure of the binding pocket of IMPDH.
- 5. A crystalline molecule or molecular complex comprising an IMPDH binding pocket defined by the structural coordinates of IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455 according to Table 7 or a homologue of said molecule or molecular complex.
- 6. A crystalline molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-432 and 449-455, according to Table 7, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has an amino acid sequence identity for the corresponding binding pocket residues of 60% or greater relative to the *S. pyogenes* IMPDH binding pocket.

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7. A crystalline IMPDH molecule defined by structural coordinates for IMPDH amino acids from *S. pyogenes* IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455.

- 8. A crystalline IMPDH molecule having (inosine monophosphate) IMP in its binding pocket.
- 15. A computer generated representation of a molecule or molecular complex comprising a binding pocket defined by the following structural coordinates of *S. pyogenes* IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455.